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Technical Memorandum No. NMC-TM-63-8

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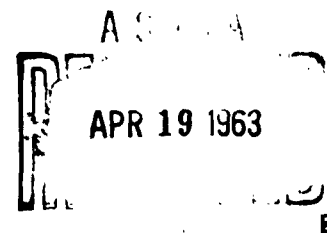


**A GENERALIZED ERROR FUNCTION
IN n DIMENSIONS**

By

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12 April 1963



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NMC Technical Memorandum NMC-TM-63-8

Published by Editorial Division
Technical Information Department
First printing 65 copies
Security classification..... UNCLASSIFIED

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SUMMARY

The error function, which occurs in much of the literature of mathematics, physics, and engineering, is generalized to handle the normal probability distribution in n dimensions.

Explicit integral representations for these functions are found to be of two general forms, depending upon whether n is even or odd.

Some readily established recursion formulas and other relationships are derived for these functions.

INTRODUCTION

The mathematical theory of probability and the related techniques of statistics are being used by an increasing number of workers in many diverse fields embracing the sciences and engineering, as well as mathematics.

Of particular importance, therefore, to engineers, to operations and systems analysts, and to the designers of experiments are certain standard probability distributions. The most widely employed of the continuous distributions is undoubtedly the "Gaussian," or "normal" distribution, which is of enormous theoretical, historical, and practical importance.

The normal distribution, with zero mean, is given by

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}} \quad (1)$$

and is completely specified by the parameter σ , called the "standard deviation."

This distribution has been generalized to n dimensions. The most general n -dimensional normal distribution contains parameters to account for nonzero means for the n independent variables, for correlations among the variables, and for unequal standard deviations with respect to each of the n variables.

This report will concern itself with a very special case of the n -dimensional distribution. In particular, the means will all be assumed zero, the correlations will all be assumed zero, and the standard deviations will be assumed equal. The resulting probability distribution is then given by

$$p(x_1, x_2, \dots, x_n) = \frac{1}{(2\pi)^{\frac{n}{2}} \sigma^n} e^{-\frac{x_1^2 + \dots + x_n^2}{2\sigma^2}} \quad (2)$$

In the one-dimensional case, a commonly occurring expression containing $p(x)$ is that for the probability with which

$$|x| \leq \alpha$$

This expression is (for $\alpha \geq 0$)

$$\text{Prob } \{-\alpha \leq x \leq \alpha\} = \int_{-\alpha}^{\alpha} p(x) dx \quad (3)$$

$$= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\alpha}^{\alpha} e^{-\frac{x^2}{2\sigma^2}} dx \quad (3)$$

$$= \frac{1}{\sigma} \sqrt{\frac{2}{\pi}} \int_0^{\alpha} e^{-\frac{x^2}{2\sigma^2}} dx \quad (\text{since the integrand is even})$$

$$= \frac{2}{\sqrt{\pi}} \int_0^{\frac{\alpha}{\sigma\sqrt{2}}} e^{-y^2} dy$$

This expression cannot be evaluated in closed form for an arbitrary upper limit, but occurs so frequently that its values have been tabulated, and the expression itself has been given the name of "error function."

The customary definition of the error function is

$$\text{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy \quad (4)$$

In terms of this definition, it follows that

$$\text{Prob} \{ |x| \leq \alpha \} = \text{erf} \left(\frac{\alpha}{\sigma\sqrt{2}} \right) \quad (5)$$

The analog of the problem in n dimensions presents no new problems in rectangular coordinates, since

$$\begin{aligned} \text{Prob} \{ |x_1| \leq \alpha_1, |x_2| \leq \alpha_2, \dots, |x_n| \leq \alpha_n \} \\ = \text{erf} \left(\frac{\alpha_1}{\sigma\sqrt{2}} \right) \text{erf} \left(\frac{\alpha_2}{\sigma\sqrt{2}} \right) \dots \text{erf} \left(\frac{\alpha_n}{\sigma\sqrt{2}} \right) \end{aligned} \quad (6)$$

as a consequence of the appropriate integral separating into a product of integrals with respect to one variable.

Something new does arise, however, from regarding $\vec{r} = (x_1, \dots, x_n)$ as a vector in n dimensions, and asking what is

$$\text{Prob} \{ |\vec{r}| \leq \alpha \}$$

This is a very natural question to ask for the cases $n = 2, 3$.

It is the purpose of the present paper to investigate this question. The result, as will be seen, is to define an "error function" generalized to n dimensions, in terms of which the required probability can be written in a manner analogous to equation (5).

Some simple properties of these generalized error functions are proved, and graphs of these functions are presented.

THE SPECIAL CASE OF TWO DIMENSIONS

As a natural way of introducing generalized error functions it is instructive to consider the case of two dimensions. This case is well known among the users of probability theory because of its frequent occurrence and the fact that the mathematics fortuitously permits a solution in closed form.

The two-dimensional treatment, moreover, is capable of a direct generalization to n dimensions, as will be seen later, and it is therefore profitable to dwell at some length upon this special case. This will now be done.

Introduce polar coordinates (r, θ) . Then

$$\begin{aligned}
 \text{Prob } \{ |\vec{r}| \leq \alpha \} &= \iint_{\substack{\text{circle about} \\ \text{origin, radius } \alpha}} \frac{1}{2\pi\sigma^2} e^{-\frac{x^2+y^2}{2\sigma^2}} dx dy \\
 &= \int_0^\alpha \int_0^{2\pi} \frac{1}{2\pi\sigma^2} e^{-\frac{r^2}{2\sigma^2}} r dr d\theta \\
 &= \int_0^\alpha \frac{1}{\sigma^2} e^{-\frac{r^2}{2\sigma^2}} r dr \\
 &= \int_{r=0}^\alpha e^{-\frac{r^2}{2\sigma^2}} d\left(\frac{r^2}{2\sigma^2}\right) \\
 &= -e^{-\frac{r^2}{2\sigma^2}} \Bigg|_{r=0}^\alpha
 \end{aligned} \tag{7}$$

$$\therefore \text{Prob } \{ |\vec{r}| \leq \alpha \} = 1 - e^{-\frac{\alpha^2}{2\sigma^2}} \tag{8}$$

This is a well known expression which appears very frequently in the literature.

The above result suggests defining an error function in two dimensions by

$$\text{erf}_2(x) = 1 - e^{-x^2} \tag{9}$$

Then

$$\text{Prob } \{ |\vec{r}| \leq \alpha \} = \text{erf}_2\left(\frac{\alpha}{\sigma\sqrt{2}}\right) \tag{10}$$

in two dimensions, analogously to equation (5).

The above computational procedure will now be extended to an n -dimensional distribution. It will be seen later that all the even-dimensional error functions are expressible in closed form, although not always conveniently so.

THE GENERAL CASE OF n DIMENSIONS

The case of n dimensions, for $n \geq 2$, is carried out analogously to the above two-dimensional treatment.

It is necessary to evaluate the following expression:

$$\text{Prob } \{ |\vec{r}| \leq \alpha \} = \iiint_{\substack{\text{hypersphere} \\ \text{about origin,} \\ \text{radius } \alpha}} \frac{1}{(2\pi)^{\frac{n}{2}} \sigma^n} e^{-\frac{x_1^2 + \dots + x_n^2}{2\sigma^2}} dx_1 \dots dx_n \tag{11}$$

The integration is simplified by introducing hyperspherical coordinates, $(R, \theta_1, \theta_2, \dots, \theta_{n-1})$, according to the transformation equations

$$\left\{ \begin{array}{llll} x_1 & = R \sin \theta_1 \sin \theta_2 & \dots & \sin \theta_{n-2} \sin \theta_{n-1} \\ x_2 & = R \sin \theta_1 \sin \theta_2 & \dots & \sin \theta_{n-2} \cos \theta_{n-1} \\ x_3 & = R \sin \theta_1 \sin \theta_2 & \dots & \sin \theta_{n-3} \cos \theta_{n-2} \\ x_4 & = R \sin \theta_1 \sin \theta_2 \dots \sin \theta_{n-4} \cos \theta_{n-3} & & \\ & \dots & & \\ x_{n-1} & = R \sin \theta_1 \cos \theta_2 & & \\ x_n & = R \cos \theta_1 & & \end{array} \right. \quad (12)$$

Equation (11) then becomes

$$\text{Prob} \{ |\vec{r}| \leq \alpha \} = \frac{1}{(2\pi)^{\frac{n}{2}} \sigma^n} \int_0^\alpha e^{-\frac{R^2}{2\sigma^2}} R^{n-1} dR \int \dots \int d\Omega_n \quad (13)$$

where $d\Omega_n$ is an element of hypersolid angle and is independent of R and dR .

In particular,

$$1 = \text{Prob} \{ |\mathbf{r}^*| < \alpha \} = \frac{1}{(2\pi)^{\frac{n}{2}} \sigma^n} \int_0^\infty e^{-\frac{R^2}{2\sigma^2}} R^{n-1} dR \int \dots \int d\Omega_n \quad (14)$$

It follows that

$$\int \dots \int d\Omega_n = \frac{(2\pi)^{\frac{n}{2}} \sigma^n}{\int_0^\infty e^{-\frac{R^2}{2\sigma^2}} R^{n-1} dR} \quad (15)$$

Substituting into equation (13),

$$\text{Prob} \{ |\mathbf{r}| \leq \alpha \} = \frac{\int_0^\alpha e^{-\frac{R^2}{2\sigma^2}} R^{n-1} dR}{\int_0^\infty e^{-\frac{R^2}{2\sigma^2}} R^{n-1} dR} \quad (16)$$

An obvious change of variable in the integrals gives the result

$$\text{Prob} \{ |\mathbf{r}'| \leq \alpha \} = \frac{\int_0^{\frac{\alpha}{\sigma\sqrt{2}}} e^{-u^2} u^{n-1} du}{\int_0^\infty e^{-u^2} u^{n-1} du} \quad (17)$$

Now define a generalized n-dimensional error function, $\text{erf}_n(x)$, by

$$\text{erf}_n(x) \equiv \frac{\int_0^x e^{-u^2} u^{n-1} du}{\int_0^\infty e^{-u^2} u^{n-1} du} \quad (18)$$

Equations (17) and (18) then imply that

$$\text{Prob} \{ |\vec{r}| \leq \alpha \} = \text{erf}_n \left(\frac{\alpha}{\sigma\sqrt{2}} \right) \quad (19)$$

which is analogous to equation (5), and is valid for $n = 1, 2, 3, 4, \dots$

For $n = 1, 2$, the definition (18) reduces to the definitions (4) and (9), respectively.

SOME FURTHER ANALYSIS

Consider the integral

$$I_k \equiv \int_0^\infty e^{-u^2} u^k du \quad (20)$$

which is used as a normalizing factor in equation (18).

Integrating by parts, it is readily established that

$$I_{k+2} = \frac{k+1}{2} I_k \quad (21)$$

It follows by mathematical induction that

$$I_{2m+1} = m! I_1 \quad ; m = 0, 1, 2, \dots \quad (22)$$

and

$$I_{2m} = \frac{(2m)!}{2^{2m} m!} I_0 \quad ; m = 0, 1, 2, \dots \quad (23)$$

but

$$I_1 = \int_0^\infty e^{-u^2} u du = \frac{1}{2} \quad (24)$$

and

$$I_0 = \int_0^\infty e^{-u^2} du = \frac{1}{2} \sqrt{\pi} \quad (25)$$

so that

$$I_{2m+1} = \frac{1}{2} m! \quad (26)$$

and

$$I_{2m} = \frac{(2m)! \sqrt{\pi}}{2^{2m+1} m!} \quad (27)$$

The definition (18) can therefore be written

$$\operatorname{erf}_{2m+1}(x) = \frac{2^{2m+1} m!}{\sqrt{\pi} (2m)!} \int_0^x e^{-u^2} u^{2m} du \quad ; m = 0, 1, 2, \dots \quad (28)$$

and

$$\operatorname{erf}_{2m}(x) = \frac{2}{(m-1)!} \int_0^x e^{-u^2} u^{2m-1} du \quad ; m = 1, 2, 3, \dots \quad (29)$$

Equations (28) and (29) may, if desired, together be taken as the definition of the generalized error function, rather than equation (18).

The error functions will now be shown to satisfy certain relationships.

Integrate equation (28) by parts. The resulting expression simplifies to

$$\operatorname{erf}_{2m+1}(x) = \frac{(2x)^{2m+1} m! e^{-x^2}}{\sqrt{\pi} (2m+1)!} + \operatorname{erf}_{2m+3}(x) \quad ; m = 0, 1, 2, \dots \quad (30)$$

Proceeding similarly with equation (29), one gets

$$\operatorname{erf}_{2m}(x) = \frac{x^{2m} e^{-x^2}}{m!} + \operatorname{erf}_{2m+2}(x) \quad ; m = 1, 2, 3, \dots \quad (31)$$

Recalling equation (9), it follows by mathematical induction on equation (31) that

$$\operatorname{erf}_{2m}(x) = 1 - e^{-x^2} \left\{ 1 + \frac{x^2}{1!} + \frac{x^4}{2!} + \dots + \frac{x^{2(m-1)}}{(m-1)!} \right\} \quad ; m = 0, 1, 2, \dots \quad (32)$$

Equation (32) shows that all the even-dimensional error functions are expressible in closed form, although for sufficiently large m the closed form expressions become increasingly complicated.

It follows also from equation (32) that

$$1 - e^{-x^2} > \operatorname{erf}_2(x) > \operatorname{erf}_4(x) > \operatorname{erf}_6(x) > \dots \quad (33)$$

and that for any preassigned x ,

$$\lim_{m \rightarrow \infty} \text{erf}_{2m}(x) = 0 \quad (34)$$

In a similar manner, mathematical induction applied to equation (30) gives the result

$$\text{erf}_{2m+1}(x) = \text{erf}(x) - \frac{e^{-x^2}}{\sqrt{\pi}} \left\{ \frac{(2x)^0 0!}{1!} + \frac{(2x)^3 1!}{3!} + \dots + \frac{(2x)^{2m-1} (m-1)!}{(2m-1)!} \right\}; \quad (35)$$

$m = 1, 2, 3, \dots$

Since $\text{erf}_1(x) = \text{erf}(x)$ cannot be expressed in closed form, neither can the odd-dimensional error functions.

However, it is clear from equation (35) that

$$\text{erf}(x) = \text{erf}_1(x) \geq \text{erf}_3(x) \geq \text{erf}_5(x) \geq \dots \quad (36)$$

since x was assumed non-negative in the definition, equation (18), in view of the probability application with regard to which the generalized error functions were introduced.

From the point of view of the pure mathematician, it is, of course, desirable to use the definition, equation (18), for negative values of x , as well as for positive values. If that is done, then the odd-dimensional error functions turn out to be odd functions, while the even-dimensional functions are even.

$$\text{i.e., } \begin{cases} \text{erf}_{2m}(x) = \text{erf}_{2m}(-x) \\ \text{erf}_{2m+1}(x) = -\text{erf}_{2m+1}(-x) \end{cases} \quad (37)$$

if x is permitted to become negative. For negative x , the inequalities (36) will all be reversed.

These error functions are plotted in figure 1 for positive arguments and dimensions up to 10.

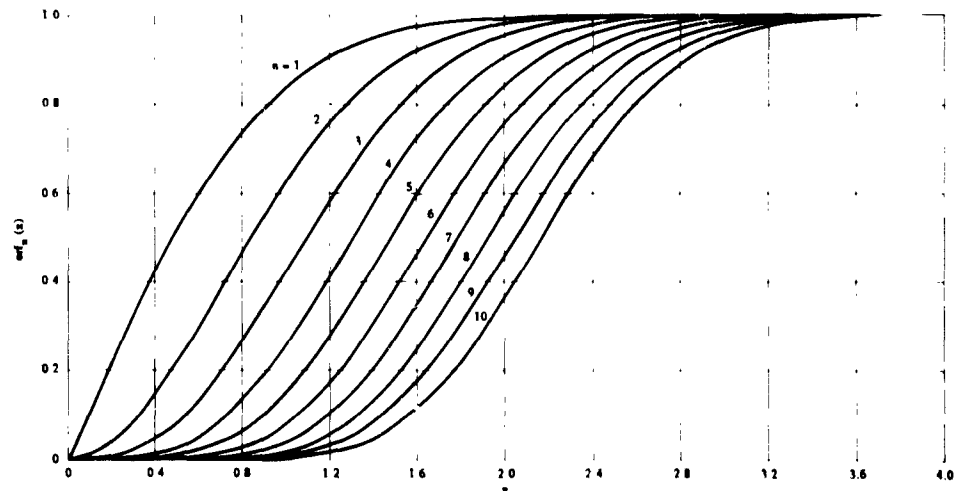


Figure 1. Generalized Error Functions, $\text{erf}_n(x)$.

APPLICATION TO HYPERELLIPSOIDAL DISTRIBUTIONS

Retaining the assumptions of zero bias and zero correlations, but allowing the standard deviations to take on the unequal values $\sigma_1, \sigma_2, \dots, \sigma_n$, equation (2) generalizes to

$$p(x_1, \dots, x_n) = \frac{1}{(2\pi)^{\frac{n}{2}} \sigma_1 \dots \sigma_n} e^{-\left(\frac{x_1^2}{2\sigma_1^2} + \dots + \frac{x_n^2}{2\sigma_n^2}\right)} \quad (38)$$

The loci along which $p(x_1, \dots, x_n)$ is constant are given by

$$\frac{x_1^2}{\sigma_1^2} + \dots + \frac{x_n^2}{\sigma_n^2} = u^2, \quad \text{a constant.} \quad (39)$$

These loci thus form a family of hyperellipsoids, centered at the origin, with semiaxes equal to $u\sigma_1, u\sigma_2, \dots, u\sigma_n$, and consequently the distribution given by equation (38) may be thought of as a hyperellipsoidal distribution.

Consider now the probability that a random vector $\vec{r} = (x_1, \dots, x_n)$ lies within the hyperellipsoid

$$\frac{x_1^2}{\sigma_1^2} + \dots + \frac{x_n^2}{\sigma_n^2} = \beta^2 : \quad (40)$$

$$\text{Prob} \left\{ \sum_i \frac{x_i^2}{\sigma_i^2} \leq \beta^2 \right\} = \iiint_{\text{hyperellipsoid}} p(\vec{r}) dV \quad (41)$$

where dV is an element of hypervolume in the n -dimensional space.

$$\therefore \text{Prob} \left\{ \sum_i \frac{x_i^2}{\sigma_i^2} \leq \beta^2 \right\} = \iiint_{\text{hyperellipsoid}} \frac{e^{-\frac{1}{2}\left(\frac{x_1^2}{\sigma_1^2} + \dots + \frac{x_n^2}{\sigma_n^2}\right)}}{(2\pi)^{\frac{n}{2}} \sigma_1 \dots \sigma_n} dx_1 \dots dx_n \quad (42)$$

$$= \iiint_{\text{hypersphere } \sum \lambda_i^2 = \beta^2} \frac{1}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2}(\lambda_1^2 + \dots + \lambda_n^2)} d\lambda_1 \dots d\lambda_n \quad (43)$$

where

$$\lambda_i = \frac{x_i}{\sigma_i}; i = 1, 2, \dots, n \quad (44)$$

$$\therefore \text{Prob} \left\{ \sum_{i=1}^n \frac{x_i^2}{\sigma_i^2} \leq \beta^2 \right\} = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_0^{\beta} R^{n-1} e^{-\frac{R^2}{2}} dR \int \dots \int d\Omega_n \quad (45)$$

introducing hyperspherical polar coordinates, as before.

Again, remembering that

$$\text{Prob} \left\{ \sum_{i=1}^n \frac{x_i^2}{\sigma_i^2} < \infty \right\} = 1 = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_0^{\infty} R^{n-1} e^{-\frac{R^2}{2}} dR \int \dots \int d\Omega_n \quad (46)$$

it follows that

$$\text{Prob} \left\{ \sum_{i=1}^n \frac{x_i^2}{\sigma_i^2} \leq \beta^2 \right\} = \frac{\int_0^{\beta} R^{n-1} e^{-\frac{R^2}{2}} dR}{\int_0^{\infty} R^{n-1} e^{-\frac{R^2}{2}} dR} = \frac{\int_0^{\frac{\beta}{\sqrt{2}}} u^{n-1} e^{-u^2} du}{\int_0^{\infty} u^{n-1} e^{-u^2} du}$$

i.e.,

$$\text{Prob} \left\{ \sum_{i=1}^n \frac{x_i^2}{\sigma_i^2} \leq \beta^2 \right\} = \text{erf}_n \left(\frac{\beta}{\sqrt{2}} \right) \quad (47)$$

Equation (47) is the desired generalization of equation (19) to the case in which the components of \vec{r} have unequal standard deviations.

It is to be noted that the dimensionless quantity β appearing in equation (47) reduces to the quantity $\frac{\lambda}{\sigma}$ of equation (19) for the special case in which $\sigma_1 = \sigma_2 = \dots = \sigma_n = \sigma$.

RECAPITULATION

The error function, which occurs in much of the literature of mathematics, physics, and engineering, has been generalized to handle the normal probability distribution in n dimensions.

Explicit integral representations for these functions were found to be of two general forms, depending upon whether n is even or odd.

Some readily established recursion formulas and other relationships were derived for these functions.